

# Computational study of atomic mobility for bcc phase in Ti–Al–Fe system

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## ABSTRACT

Experimental diffusion data were critically assessed to develop the atomic mobility for the bcc phase of the Ti–Al–Fe system by using the DICTRA software. Good agreements were obtained from comprehensive comparisons made between the calculated and the experimental diffusion coefficients. The developed atomic mobility was then validated by well predicting the interdiffusion behavior observed from the diffusion-couple experiments in available literature.

## 1. Introduction

High specific strength reached by  $\beta$ -titanium alloys, along with extraordinary corrosion resistance and biocompatibility, boosts them with widespread applications in aerospace, automotive and healthcare industries [1,2]. Though progress seen, high-cost of the  $\beta$ -Ti alloys limits their applications, which could be reduced by substituting the expensive  $\beta$ -stabilizers Mo, V by cheaper elements like Fe. The substitution has attracted extensive research efforts on the Ti–Al–Fe based  $\beta$  alloys such as Timetal LCB (Ti–1.5Al–4.5Fe–6.8Mo) and Timetal 125 (Ti–2.7Al–5.7Fe–6V–6Mo) [3]. Such  $\beta$ -Ti alloys typically exhibit complex microstructure largely resulted from recovery, recrystallization, transformation, and precipitation. Much of these processes are governed by diffusion interaction during thermomechanical and/or heat treatment process, and that in turn provides incentives to develop knowledge of diffusion kinetics for new low-cost Ti-based alloys.

Nowadays, computational thermodynamics (or called as the CALPHAD method) [4] and DICTRA-type diffusion modeling [5] have ability to predict high-quality thermodynamic and diffusion information for many commercially important alloys that contain more than a dozen elements. Due to having the atomic mobility (rather than diffusivity) as a base [5], the DICTRA-type diffusion model is particularly good for creating kinetic databases and

performing diffusion modeling for commercially important multi-component systems, because it defines one unique mobility for each component in a multicomponent system. More importantly, the mobility database can be used in conjunction with the CALPHAD-base (Calculation of Phase Diagram) thermodynamic database to obtain sufficiently reliable thermodynamic quantities, thus having the ability to offer a full diffusion picture of alloys of interest without extra experimental measurements.

So far, there are currently two commercial thermodynamic databases available for titanium alloys [6,7] that should cover the Ti–Al–Fe ternary, however, the atomic mobility of the ternary is clearly missing though the descriptions of the constituent binaries [8–11] have been developed. The objectives of the present work are therefore to assess the atomic mobility for the bcc phase of the Ti–Fe binary and then of the Ti–Al–Fe ternary by using the DICTRA software, which allows the diffusion-couple experiments and diffusion characteristics to be simulated.

## 2. Model description

According to the model suggested by Andersson and Ågren [12] and later modified by Jonsson [13], the atomic mobility  $M_i$  is expressed as

$$M_i = M_i^0 \exp\left(\frac{-Q_i^S}{RT}\right) \frac{1}{RT} m_i^* \Gamma, \quad (1)$$

where  $M_i^0$  is the frequency factor,  $Q_i^S$  is the activation energy,  $R$  is the gas constant and  $T$  is the temperature, and  $^{mg}I$  is a factor taking into account the effect of ferromagnetic ordering. The first two parts of the mobility parameter can be grouped into a single parameter, i.e.,  $Q_i = -Q_i^S + RT \ln M_i^0$  if without ferromagnetic effect. Similar to the phenomenological CALPHAD approach, the parameter  $Q_i$  is approximated to be of compositional dependence and can be expressed by the Redlich–Kister polynomial [14], i.e.,

$$Q_i = \sum_p x_p Q_i^p + \sum_p \sum_{q>p} x_p x_q \left[ \sum_{r=0,1,2,\dots}^r Q_i^{p,q,r} (x_p - x_q)^r \right] + \sum_p \sum_{q>p} \sum_{v>q} x_p x_q x_v [v_{pqv}^s Q_i^{p,q,v}], \quad (S=p, q, v), \quad (2)$$

where  $x_p$  is the mole fraction of species  $p$ ,  $Q_i^p$  is the value  $Q_i$  of species  $i$  in pure species  $p$ ,  $^r Q_i^{p,q}$  and  $^r Q_i^{p,q,v}$  are the binary and ternary interaction parameters.

The ferromagnetic effect is not negligible in the Ti–Al–Fe bcc alloys, which invariably leads to a diffusion rate lower than what is simply extrapolated from the paramagnetic state. To incorporate this effect, Jonsson [15] suggested to split the total activation energy  $Q_k$  for diffusion in a paramagnetic contribution  $Q_k^p$  and a ferromagnetic contribution  $\Delta Q_k^{mg}$ :

$$Q_k = Q_k^p + \Delta Q_k^{mg}. \quad (3)$$

The ferromagnetic contribution is

$$\Delta Q_k^{mg} = \left[ \alpha_{mg}^{mg} \Delta H \left( \frac{6}{Q_k^p} - \frac{1}{RT} \right) \right], \quad (4)$$

$^{mg} \Delta H$ , the magnetic enthalpy, is defined according to the Hillert–Jarl [16] model and  $\alpha$  is a factor of proportionality. The optimized value of  $\alpha_{mg}$  for substitutional diffusion in Fe and other bcc metals in general is 0.3 [15], which is adopted in this work.

All diffusivities can be related to the atomic mobility, e.g., the tracer diffusivity  $D_i^*$  is directly related to the atomic mobility by a simple relation:

$$D_i^* = RT M_i, \quad (5)$$

and the interdiffusion coefficient  $\tilde{D}_{pq}^n$  ( $n$  as dependent species) can be derived as

$$\tilde{D}_{pq}^n = \sum_{i=1}^{n-1} (\delta_{ip} - x_p) x_i M_i \left( \frac{\partial \mu_i}{\partial x_q} - \frac{\partial \mu_i}{\partial x_n} \right), \quad (6)$$

where the Kronecker delta  $\delta_{ip} = 1$  when  $i=p$  and 0 otherwise, and  $\mu_i$  is the chemical potential of species  $i$ . Upon the proposed relations, the mobility parameters,  $Q_i^p$ ,  $^r Q_i^{p,q}$  and  $^r Q_i^{p,q,v}$ , can be numerically assessed by fitting to experimental diffusion coefficients.

The composition, varying with the diffusion time  $t$  in the diffusion zone of diffusion couple, can be described by the equation of continuity

$$\frac{1}{V_m} \frac{\partial x_i}{\partial t} + \nabla \cdot \tilde{J}_i = 0, \quad (7)$$

where  $V_m$  is the molar volume which is generally treated as a constant, and  $\tilde{J}_i$  is the interdiffusion flux. With different initial conditions and boundary conditions, Eq. (7) can be solved numerically to express the form of the concentration profile.

### 3. Evaluation of experimental diffusion data

The experimental diffusion data accepted in this work to assess the mobility includes the tracer, impurity, and interdiffusion coefficients [17–23]. In the subsections that follow, the data are evaluated system by system.

**Table 1**  
Assessed atomic mobilities for the BCC phase of the Ti–Al–Fe ternary system.

Mobility	Parameter (J/mole)	Reference
<b>Mobility of Al</b>		
$Q_{Al}^{Al}$	$-215,000 - 80.2 \times T$	[28]
$Q_{Al}^{Fe}$	$-215,000 - 80.2 \times T$	[28]
$Q_{Al}^{Ti}$	$R \times T \times \ln[5.51E - 6 \times \exp(-204,000/T/R) + 5.19E - 10 \times \exp(-96,000/T/R)]$	[9]
$^0 Q_{Al}^{Al,Fe}$	$-103,042.84$	Present work
$^1 Q_{Al}^{Al,Fe}$	$-138,569.51$	Present work
$^0 Q_{Al}^{Al,Ti}$	$-429,380.7 + 44.5 \times T$	Present work
$^1 Q_{Al}^{Al,Ti}$	$-344,886 - 124.5 \times T$	Present work
$^0 Q_{Al}^{Ti,Fe}$	$200,000$	Present work
<b>Mobility of Fe</b>		
$Q_{Fe}^{Al}$	$-218,000 - 83.036 \times T$	[28]
$Q_{Fe}^{Fe}$	$-218,000 - 83.036 \times T$	[28]
$Q_{Fe}^{Ti}$	$R \times T \times \ln[7.8E - 7 \times \exp(-132,000/T/R) + 2.7E - 4 \times \exp(-230,300/T/R)]$	[19]
$^0 Q_{Fe}^{Al,Fe}$	$155,103.69$	Present work
$^1 Q_{Fe}^{Al,Fe}$	$52,711$	Present work
$^0 Q_{Fe}^{Ti,Fe}$	$-393,647.8 + 243.2 \times T$	Present work
$^1 Q_{Fe}^{Ti,Fe}$	$325,715.5 - 243.5 \times T$	Present work
$^0 Q_{Fe}^{Ti,Al}$	$-70,000$	Present work
<b>Mobility of Ti</b>		
$Q_{Ti}^{Al}$	$-199,404.05 - 90.78 \times T$	[9]
$Q_{Ti}^{Fe}$	$-183,366.04 - 93.54 \times T$	Present work
$Q_{Ti}^{Ti}$	$R \times T \times \ln[5.91E - 5 \times \exp(-237,000/T/R) + 1.47E - 8 \times \exp(-121,000/T/R)]$	[26]
$^0 Q_{Ti}^{Ti,Fe}$	$-83,923.7$	Present work
$^0 Q_{Ti}^{Ti,Al}$	$-103,961.05 + 116.6 \times T$	Present work
$^1 Q_{Ti}^{Ti,Al}$	$280,172.98 - 157.8 \times T$	Present work

### 3.1. The Ti-Fe binary

By means of the serial sectioning method, Klugkist and Herzig [17] measured the tracer diffusivity of Ti in pure bcc-Fe over the temperature range of 948–1174 K by using the isotope  $^{44}\text{Ti}$ . The magnetic effect was observed that deviates the Arrhenius plot of the Ti impurity diffusion in bcc-Fe from a linear relation. Likewise, the tracer diffusivities of Fe in bcc-Ti was investigated by Gibbs et al. and those in the Ti-Fe (0–15 at% Fe) binary alloys by Peart and Tomlin [18]. The tracer diffusion experiment and Mossbauer spectroscopy in the bcc Ti-Fe alloys undertaken by Nakajima et al. [20] studied the effect of Fe on the diffusion in concentrated Ti-Fe binary alloys (0–13 at% Fe) and the diffusion mechanism. Concerning the interdiffusion coefficients in the bcc Ti-Fe alloys, Taguchi et al. [21] determined those in the temperature range of 950–1140 K by using the Ti/Fe diffusion couples while Takahashi et al. studied at higher temperatures 1423 K [22] and 1473 K [23] by the Ti/Ti–13.5Fe incremental couples.

### 3.2. The Ti-Al-Fe ternary

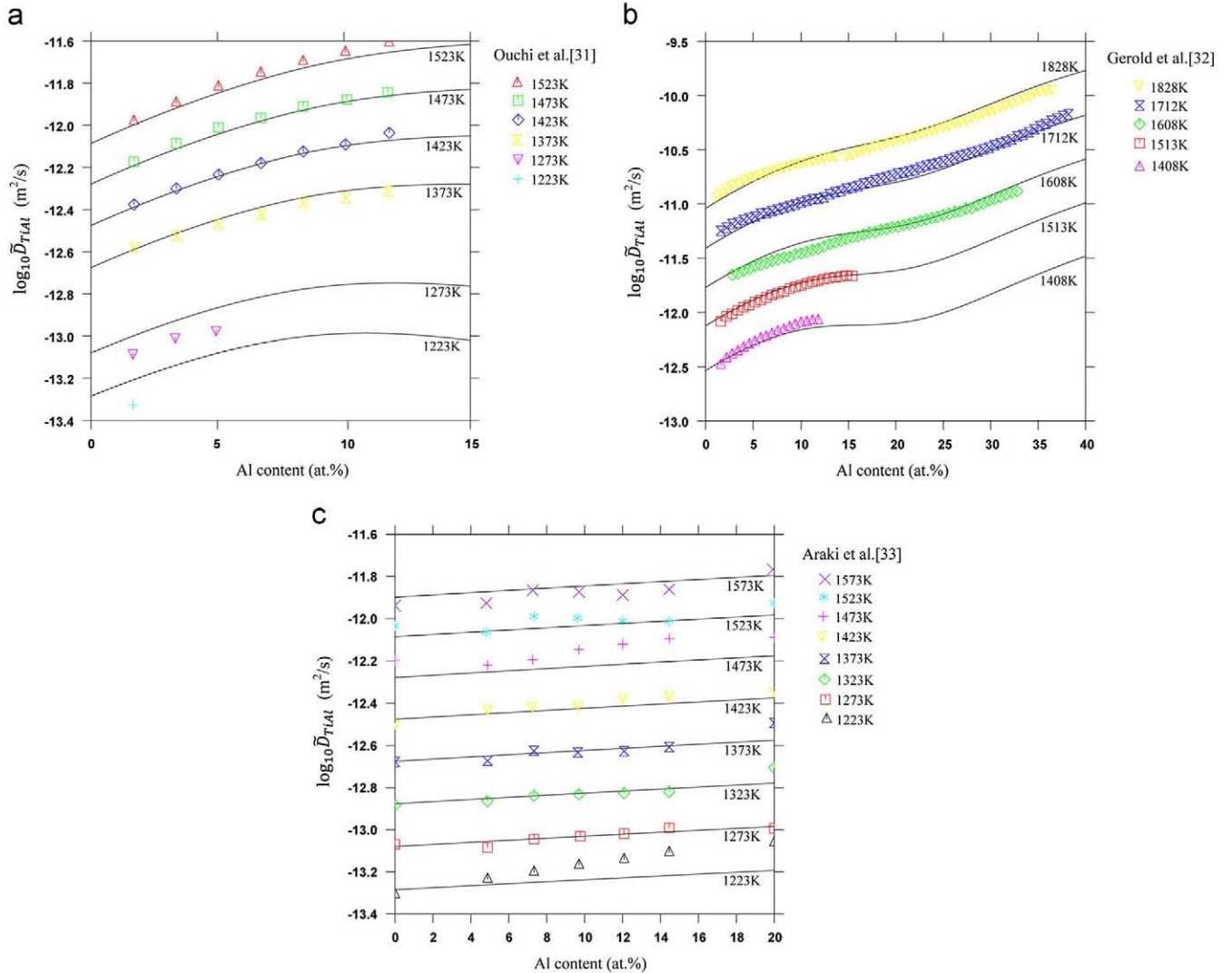
The interdiffusion and impurity coefficients have been recently determined for the bcc Ti-Al-Fe ternary alloys at the Ti-rich corner over the temperatures from 1423 K [22] to 1473 K [23]

by using the Matano–Kirkaldy and the modified Hall methods. All determined interdiffusion coefficients were examined and obey the thermodynamic constraints [24], in this work, all the main coefficients but the cross ones were used to optimize the ternary interaction parameters because the latter exhibits somewhat larger scattering.

## 4. Optimization procedure

The thermodynamic factor of diffusion can be readily computed from the CALPHAD-base thermodynamic parameters. In this work, the thermodynamic parameters of the bcc phase of the Ti-Al-Fe ternary were taken from CompuTherm [25]. The mobility of bcc-Ti self-diffusion assessed by Chen et al. [26] was accepted in this work because it excels Ref. [11] at representing the strongly curved Arrhenius law of bcc-Ti diffusion [27], yet has a clearer physical meaning than a piecewise approximation. The parameters of the Fe impurity diffusion in bcc-Ti fitted by Gibbs et al. [19] were accepted.

Recently, the mobility for the bcc Ti-Fe alloys has been assessed [29], however, one comes to realize that a reassessment is required when looking at the facts: (1) a temperature dependent activation energy was assumed to describe the Ti self-diffusion; (2) the Fe



**Fig. 1.** Calculated interdiffusion coefficients of the bcc Ti-Al alloys compared with the experimental measurements of (a) Ouchi et al. [31], (b) Gerold and Herzig [32] and (c) Araki et al. [33].



diffusion in bcc-Ti was unrealistically assumed to obey a linear Arrhenius relation; (3) the Ti diffusion in bcc-Fe is not repeatable by using the published mobility; (4) no any experimental interdiffusion data from Refs. [21–23] was included in their assessment; and (5) no validation was made for any ternary systems. Due to the uptake of different thermodynamic descriptions of Ti–Al from Huang et al. [8] and Li et al. [9] and of Al–Fe from Helander and Agren [28] and Cui et al. [34], the mobilities of the two binaries were reassessed while all the relevant self and impurity parameters [9,26,28] were kept.

All the other parameters were optimized by fitting to the selected experimental diffusion data [17–23] by using the DICTRA software [30]. The strategy of optimization is as follows: the parameter  $Q_{Ti}^{Fe}$  was optimized first by fitting to the Ti impurity diffusivity in bcc-Fe, the interaction parameters  ${}^0Q_{Fe}^{Ti,Fe}$  and  ${}^1Q_{Fe}^{Ti,Fe}$  were then obtained by describing the Fe tracer diffusion in the Ti–Fe binary alloys while  ${}^0Q_{Ti}^{Ti,Fe}$  was from the Ti–Fe interdiffusion coefficients. Following the same strategies in Ref. [8] for Ti–Al and in Ref. [34] for Al–Fe, the mobilities of the two binaries were

reassessed, which were finally used together with the Ti–Fe binary to optimize the Ti–Al–Fe ternary interaction parameters by representing the ternary diffusion data. All the mobility parameters of the Ti–Al–Fe ternary system are listed in Table 1.

## 5. Results and discussions

### 5.1. The Ti–Al and Al–Fe binary

Validation of the assessed mobility parameters can be primarily carried out by using them for deriving various diffusion coefficients. Fig. 1 presents the comparisons of the Ti–Al interdiffusion coefficients between the calculated data and experimental points [31–33]. As can be seen, general agreement is obtained when taking into account the scattering of experimental data at relatively low temperatures. Likewise, Fig. 2 shows a good agreement with the latest interdiffusion coefficients of the Al–Fe binary [34–36].

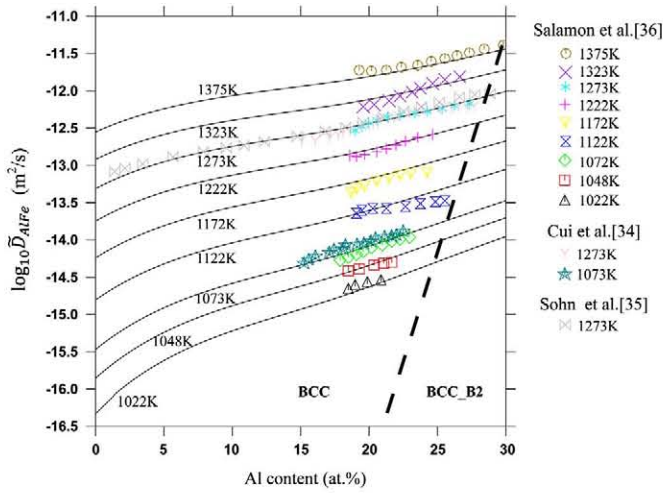


Fig. 2. Calculated interdiffusion coefficients in the bcc Al–Fe alloys compared with the experimental data (symbols).

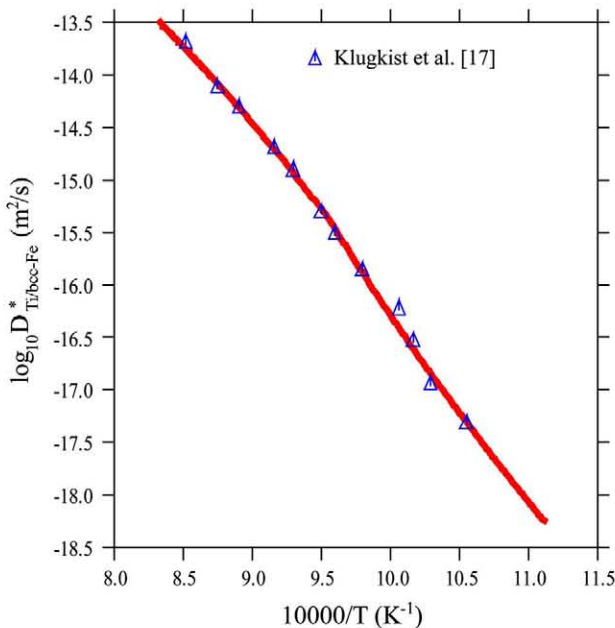


Fig. 3. Arrhenius plot of the Ti impurity diffusion in bcc-Fe. Symbols are from the experimental measurements [17].

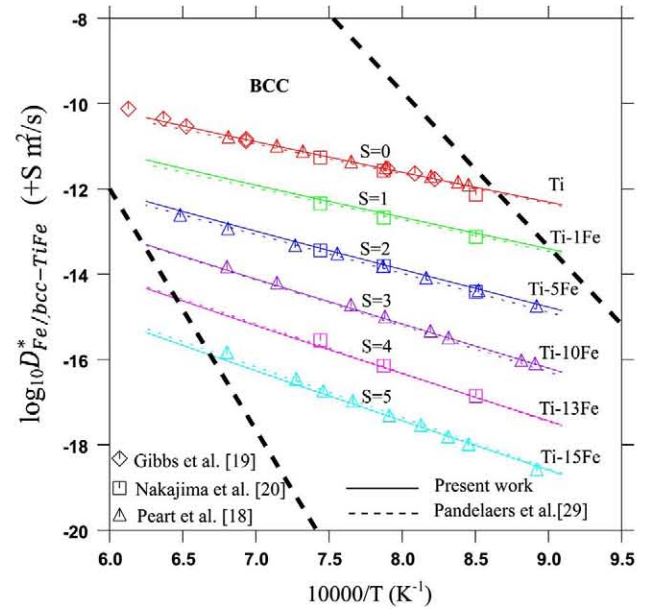


Fig. 4. Arrhenius plot of the Fe tracer diffusion in the bcc Ti–Fe alloys. Symbols are from the experimental measurements [18–20].

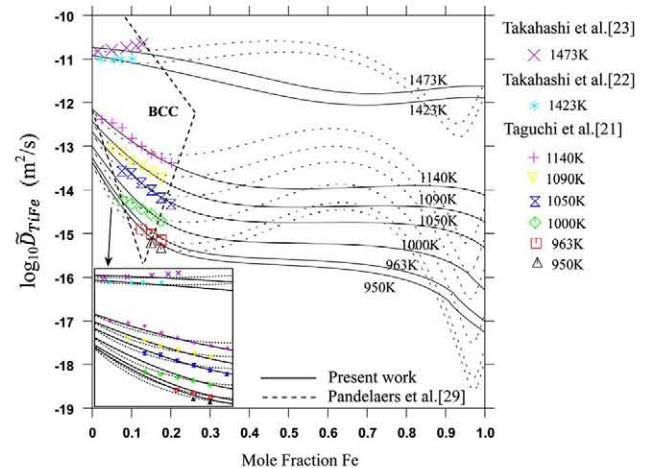


Fig. 5. The variation of the interdiffusion coefficients of the bcc Ti–Fe binary alloys in the Fe content and temperature. Symbols are from the experimental measurements [21–23].

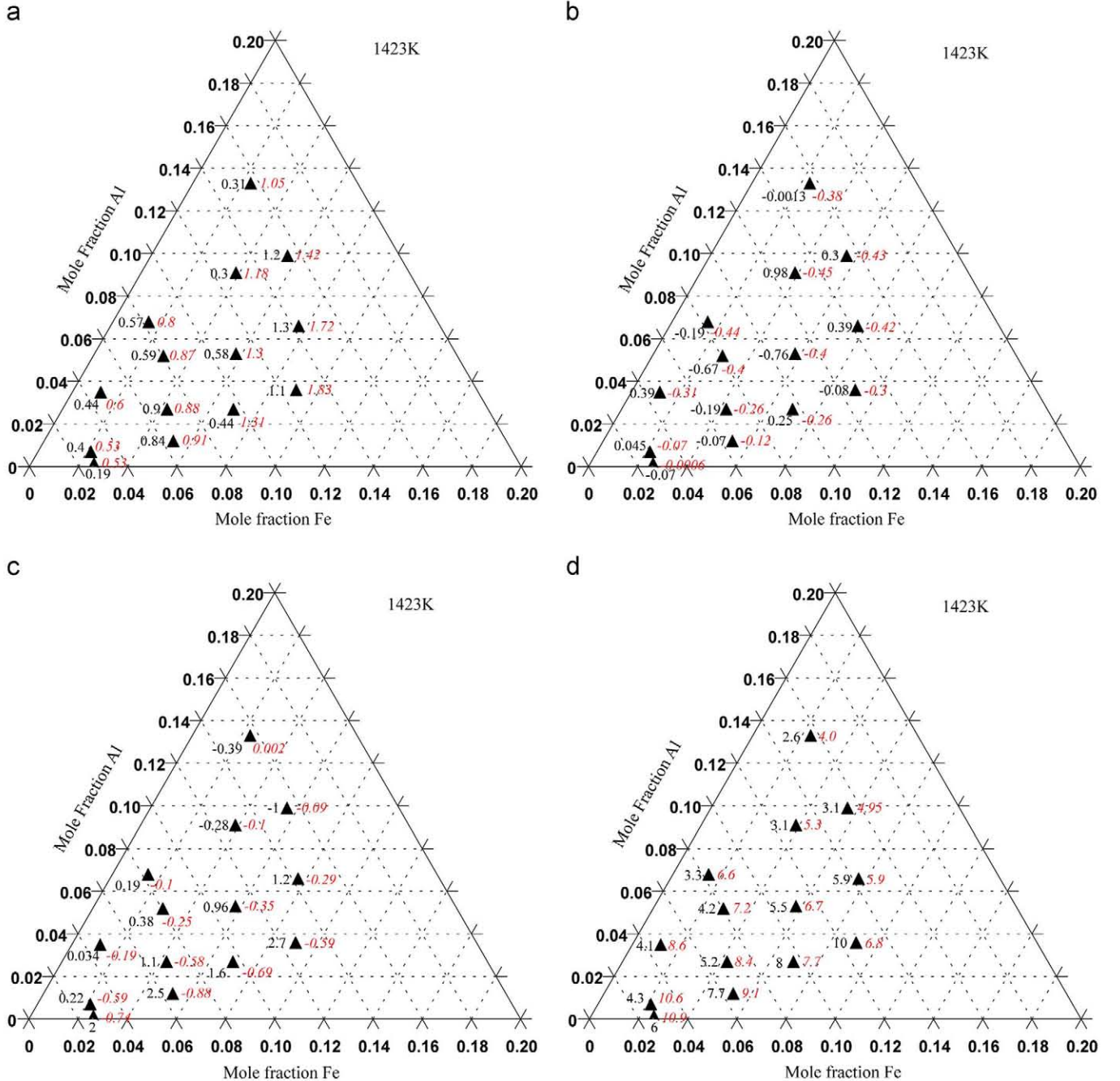
### 5.2. The Ti-Fe binary

The calculated Ti impurity diffusivity in bcc-Fe is favorably compared in Fig. 3 with the measured data from Ref. [17]. It is apparent that, like the Fe self-diffusion, the magnetic ordering results in extra suppression of the Ti diffusion below the Curie temperature. Fig. 4 presents the Arrhenius plot of the Fe tracer diffusion in the bcc Ti-Fe alloys in comparison with the measured points by Refs. [18–20], demonstrating that the Fe trace diffusivity decreases with increasing the Fe content. The calculated interdiffusion coefficients of the Ti-Fe alloys are presented in Fig. 5 with the experimental data [21–23,29] shown for comparison. Apparently, our calculation represents that the compositional dependence of the interdiffusion coefficients is weak at high

temperatures from 1423 to 1473 K, and it turns strong at the temperatures lower than 1140 K, for specific, abruptly decrease with increasing the Fe content. On the contrary, Pandelaers et al.'s assessment [29] shows the suspicious compositional dependence (see the dotted curves in Fig. 5).

### 5.3. The Ti-Al-Fe ternary

The calculated main ternary interdiffusion coefficients,  $\tilde{D}_{AlAl}^{Ti}$  and  $\tilde{D}_{FeFe}^{Ti}$ , and the cross coefficients,  $\tilde{D}_{AlFe}^{Ti}$  and  $\tilde{D}_{FeAl}^{Ti}$ , are compared with the experimental data [22,23] for 1423 K and 1473 K respectively in Figs. 6 and 7. The agreements are very reasonable, particularly good for the main coefficients. Some minor discrepancy is distinguished for the cross coefficients, which is however



**Fig. 6.** Calculated interdiffusion coefficients (in italic font) of the bcc Ti-Al-Fe ternary alloys at 1423 K in a comparison with the experimental measurement [22]: (a)  $\tilde{D}_{AlAl}^{Ti}$ , (b)  $\tilde{D}_{FeFe}^{Ti}$ , (c)  $\tilde{D}_{FeAl}^{Ti}$ , and (d)  $\tilde{D}_{AlFe}^{Ti}$ .



due to the usual scatter and relatively larger uncertainty in the experimental cross data. Note that all  $\tilde{D}_{AlFe}^{Ti}$  and  $\tilde{D}_{FeAl}^{Ti}$  cross coefficients are computed to be negative rather than abnormally changing sign of the coefficients composition by composition. To this end, our calculations allow the variation of interdiffusion coefficients in the concentration to be appropriately predicted, i.e., the Al and Fe diffusions increase in the Al gradients while decrease in the Fe gradients with increasing the Al content; by contrast, increasing the Fe content leads to a rise of the Al diffusions in the Al gradients.

#### 5.4. Simulation of diffusion couple experiments

Further validation can be performed by comparing the predicted in-depth diffusion behavior resulting from interdiffusion

with available experimental data. In conjunction with the thermodynamic database solving Eq. (7) numerically enables much of the diffusion couple experiments to be predicted. Examples of the Ti–Al–Fe ternary diffusion couples are shown for the concentration profiles of Ti/Ti–10.5Al–7.0Fe in Fig. 8(a) and Ti–3.5Al/Ti–3.5Fe in Fig. 8(b) both at 1473 K with the experimental points [23] for comparison. The agreement is apparently very satisfactory. Fig. 9 compares the simulated diffusion paths, i.e. the curves on the ternary isotherm mapping the locus of the compositions in planes parallel to the couple interface throughout the diffusion zone, with the experimental points measured from the diffusion couples at 1423 K [22] and 1473 K [23]. The agreement is good for a majority of the diffusion couples but it is not good for the G2 at 1423 K and G1, H2 at 1473 K couples. In fact, closer inspection reveals that the

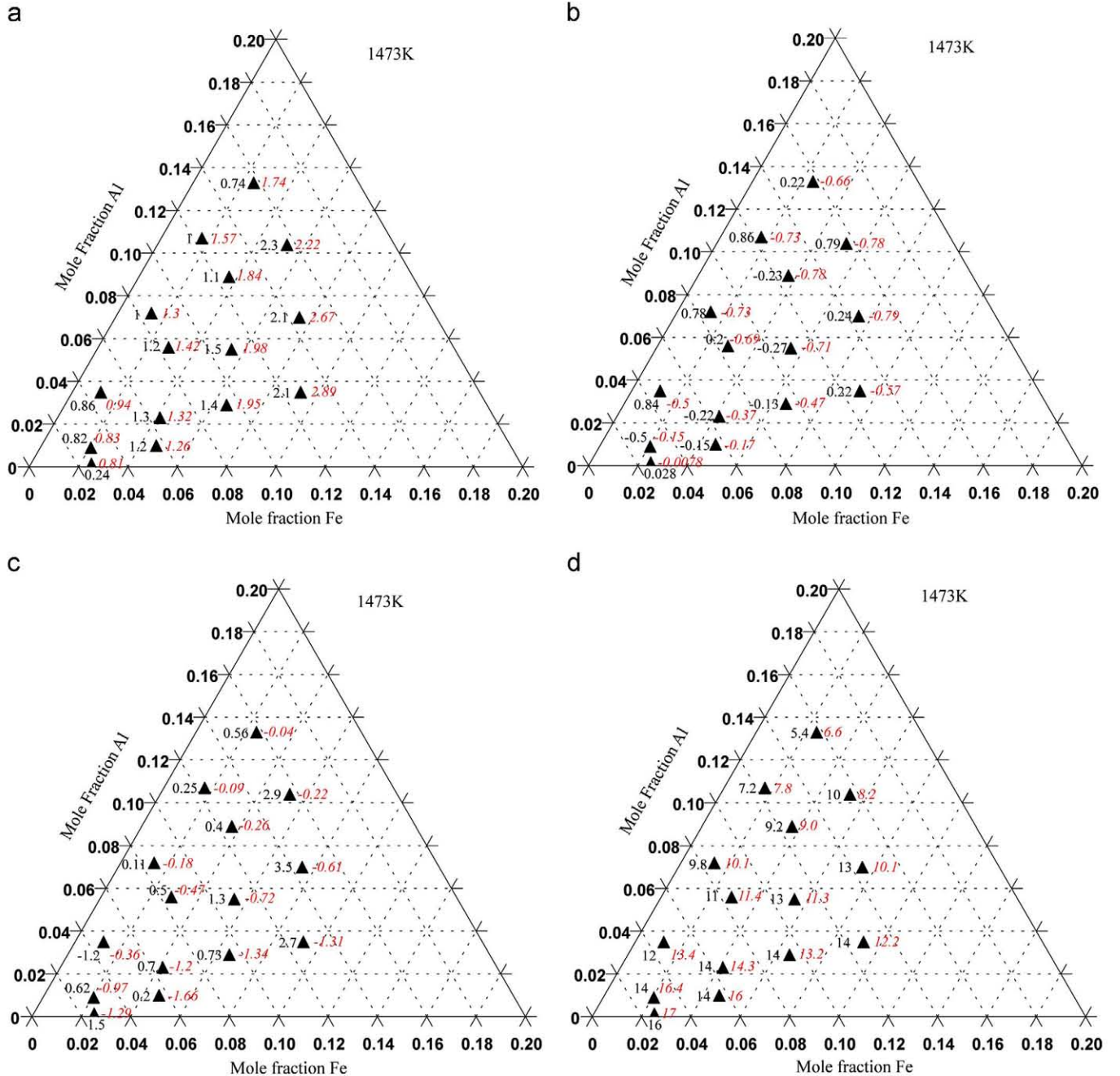


Fig. 7. Calculated interdiffusion coefficients (in italic font) of the bcc Ti–Al–Fe ternary alloys at 1473 K in a comparison with the experimental measurement [23]: (a)  $\tilde{D}_{AlAl}^{Ti}$ , (b)  $\tilde{D}_{AlFe}^{Ti}$ , (c)  $\tilde{D}_{FeAl}^{Ti}$ , and (d)  $\tilde{D}_{FeFe}^{Ti}$ .

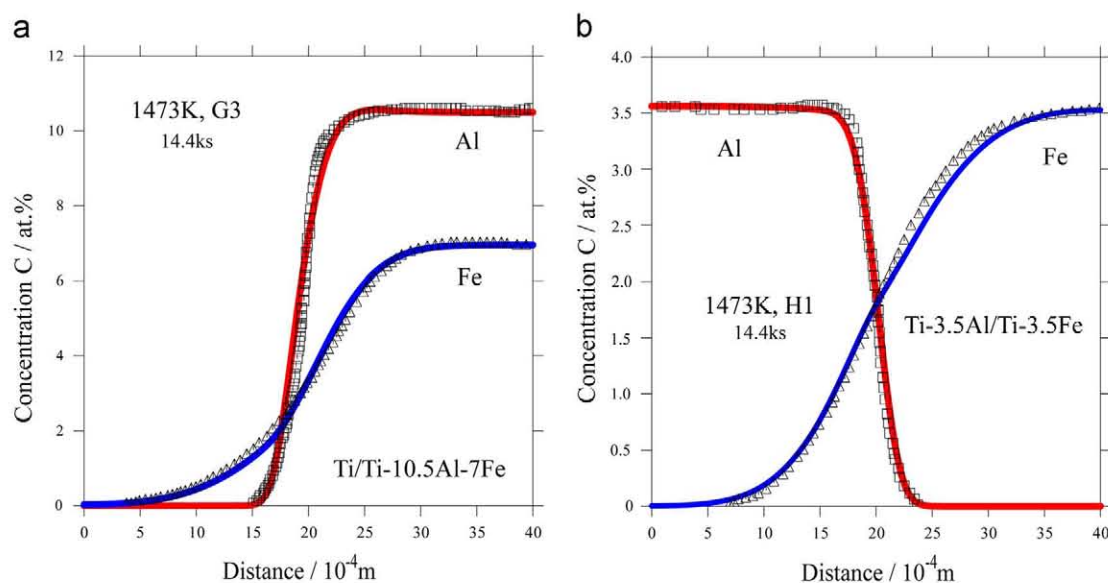


Fig. 8. Simulated concentration profiles for: (a) Ti/Ti-10.5Al-7.0Fe and (b) Ti-3.5Al/Ti-3.5Fe diffusion couples at 1473 K in a comparison with the experimental measurement [23].

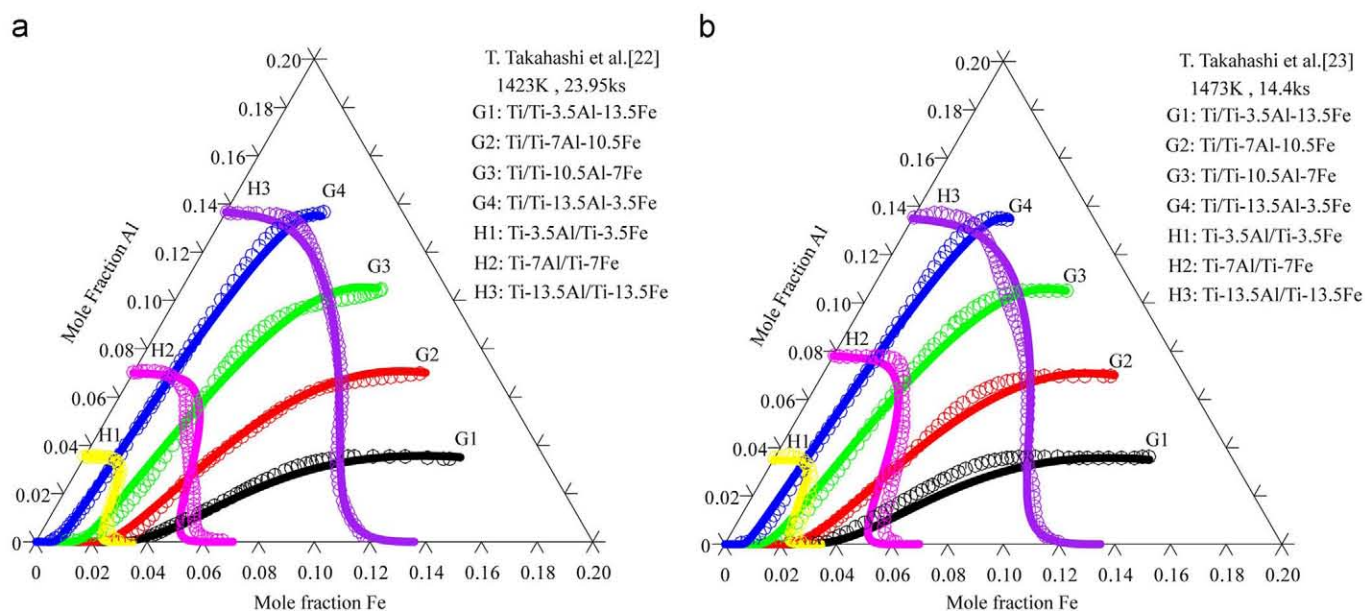


Fig. 9. Simulated diffusion paths for ternary couples at the temperatures of: (a) 1423 K and (b) 1473 K compared with the experimental measurement (symbols) [22,23].

agreement is generally good for G2 at 1473 K and G1, H2 at 1423 K, thus indicating that a comprehensive assessment of the atomic mobility of the Ti-Al-Fe ternary, together with the sub-binaries, does not allow a significant temperature dependence of the ternary diffusion data as indicated by the diffusion paths measured by Takahashi et al. [22,23] unless an unrealistically large temperature term is instead used for the optimized ternary mobility parameters.

## 6. Conclusion

The experimental diffusion data were assessed to develop the atomic mobility for the bcc phase of the Ti-Fe and the Ti-Al-Fe ternary by using the DICTRA software. General satisfactory agreements were obtained from comprehensive comparisons made between the calculated diffusion coefficients and the available experimental values. The developed atomic mobility database, in conjunction with the CALPHAD-base thermodynamic description,

has been successfully validated through further predicting a number of ternary diffusion couple experiments.

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## Appendix A. Supplementary materials

Supplementary data associated with this article can be found in the online version at: <http://dx.doi.org/10.1016/j.calphad.2014.05.004>.

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